Parity operator. Symmetric potentials and parity.

Inversion or parity operation $\Rightarrow$ reflection in space about the origin

\[ \hat{P} \begin{pmatrix} \bar{r} \end{pmatrix} = \begin{pmatrix} -\bar{r} \end{pmatrix} \]

\[ \hat{P} \psi(\bar{r}) = \psi(-\bar{r}) \]

\[ \hat{P} \] is Hermitian $\Rightarrow \int d^3r \, \psi^*(\bar{r}) \hat{P} \psi(\bar{r}) = \int d^3r \, \psi^*(-\bar{r}) \psi(-\bar{r}) = \int d^3r \, \psi^*(-\bar{r}) \psi(\bar{r}) = \int d^3r \, [\hat{P} \psi(\bar{r})]^* \psi(\bar{r})

\[ \hat{P}^+ = \hat{P} \]

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\[ \langle \psi | \hat{P}^+ | \psi \rangle \Rightarrow \hat{P}^+ = \hat{P} \]
\[ \hat{P}^2 = \hat{I} \Rightarrow \hat{P} = \hat{P}^{-1} \]

\[ \hat{P}^+ = \hat{P}^{-1} \Rightarrow \text{unitary} \]

- Eigenvalues are ±1

\[ \hat{P} \Psi_+ (\vec{r}) = \Psi_+ (-\vec{r}) = \Psi_+ (\vec{r}) \leq \text{even function} \]

\[ \hat{P} \Psi_- (\vec{r}) = \Psi_- (-\vec{r}) = -\Psi_- (\vec{r}) \leq \text{odd function} \]

So, the eigenfunctions of \( \hat{P} \) have definite parity they are either even or odd.

- \( |\Psi_+\rangle, |\Psi_-\rangle \) are orthogonal (since \( \hat{P} \) is Hermitian and

\[ <\Psi_+|\Psi_-> = \int d^3r \ \Psi_+^*(\vec{r})\Psi_- (\vec{r}) = |\Psi_+\rangle, |\Psi_-\rangle > \]

\[ = \int d^3r \ \Psi_+^* (-\vec{r}) \Psi_- (-\vec{r}) = \]

\[ = -\int d^3r \ \Psi_+^* (\vec{r}) \Psi_- (\vec{r}) = -<\Psi_+|\Psi_-> \Rightarrow 0 \]

- For any function \( \Psi(\vec{r}) \) we can construct even function \( \Psi_+ (\vec{r}) = \frac{1}{2} \left[ \Psi(\vec{r}) + \Psi(-\vec{r}) \right] \)

and odd function \( \Psi_- (\vec{r}) = \frac{1}{2} \left[ \Psi(\vec{r}) - \Psi(-\vec{r}) \right] \)
Since $\hat{P}^2 = I \quad \Rightarrow \quad \hat{P}^n = \begin{cases} \hat{P} & \text{when } n \text{ is odd} \\ I & \text{when } n \text{ is even} \end{cases}$

\[ \hat{P}^n = \underbrace{\hat{P} \hat{P} \cdots \hat{P}}_{n \text{ times}} \otimes \underbrace{\hat{I} \hat{I} \cdots \hat{I}}_{\frac{n}{2} \text{ times if } n \text{ is even}} = \hat{I} \]

\[ \Rightarrow \quad \underbrace{\hat{I} \hat{I} \cdots \hat{P}}_{\frac{n-1}{2} \text{ times if } n \text{ is odd}} = \hat{P} \]

**Even and odd operators**

\( \hat{A} \) is **even** if \( \hat{P} \hat{A} \hat{P} = \hat{A} \)

\( \hat{A} \) is **odd** if \( \hat{P} \hat{A} \hat{P} = -\hat{A} \)

For even operators \( \Rightarrow [\hat{A}, \hat{P}] = [\hat{P} \hat{A} \hat{P}, \hat{P}] = \hat{P} [\hat{P} \hat{A}, \hat{P}] = \hat{P} [\hat{P}, \hat{P}] \hat{A} + \hat{P} \hat{A} [\hat{P}, \hat{P}] = 0 \)

So, \( \hat{A}, \hat{P} \) commute

For odd operators \( \Rightarrow \hat{A} \hat{P} = -\hat{P} \hat{A} \hat{P} \hat{P} = -\hat{P} \hat{A} \)

\( \hat{A}, \hat{P} \) anti-commute
Example What is the parity of the position and momentum operators?

Consider the position operator \( \hat{R} \)

\[ \hat{R} | \vec{r} \rangle = \vec{r} | \vec{r} \rangle \]

Apply \( \hat{P} \):

\[ \hat{P} \hat{R} | \vec{r} \rangle = \hat{R} \hat{P} | \vec{r} \rangle = \hat{R} | \vec{r} \rangle = \vec{r} | -\vec{r} \rangle \]

\[ = \vec{r} | -\vec{r} \rangle \]

If apply \( \hat{P} \) first:

\[ \hat{P} | \vec{r} \rangle = | -\vec{r} \rangle ; \text{ now apply } \hat{R} \]

\[ \hat{R} \hat{P} | \vec{r} \rangle = \hat{R} | -\vec{r} \rangle = | -\vec{r} \rangle \]

\[ \hat{P} \hat{R} = -\hat{R} \hat{P} \rightarrow \text{anti-commute} \Rightarrow \hat{R} \text{ is odd} \]

Similarly, \( \hat{P} \) is odd

- For even operators \( \hat{A} \):

  \[ \hat{P} \hat{A}^n \hat{P} = \hat{A}^n \]

  \[ \Rightarrow \hat{P} \hat{A}^n \hat{P} = (-1)^n \hat{A}^n \]
Why do we care about parity? 

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Can simplify calculations

Consider symmetric (or even) potentials

\( V(x) = V(-x) \). \( \Rightarrow \) in this case, the Hamiltonian

\[
H(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)
\]

is also even,

i.e. \( H(-x) = H(x) \)

\( \downarrow \)

\( P \) is odd,

but \( P^2 \) is even.

\( H \) and \( P \) commute \( \Rightarrow \) share an eigenbasis

- Consider non-degenerate spectrum

In the case of bound states (discrete spectrum)

in 1D

Since \( P \) has eigenstates of definite parity \( \Rightarrow \)

the bound states (eigenstates of \( H \)) also have definite parity \( i.e. \) they are either even or odd

\( V(-x) = V(x) \) \( \Rightarrow \) \( \Psi(-x) = \pm \Psi(x) \)

So, for any symmetric 1D potential \( \Rightarrow \) have two families of solutions \( \Rightarrow \) even

odd
Degenerate spectrum
In this case the eigenfunctions do not have definite parity

See Sakurai pp. 274-276 for discussion
256-258 < gray (newest) edition
< red book

Parity selection rule

Consider \( 1x >, 1\beta > \) \( \in \) parity operator

\( P|x > = \varepsilon_x |x >, \ P|\beta > = \varepsilon_\beta |\beta > \)

\( \varepsilon_x , \varepsilon_\beta = \pm 1 \)

Then \( \langle \beta | \bar{R} |x > = \frac{\langle \beta | P^{-1} \bar{P} \bar{R} P^{-1} P |x >}{\varepsilon_\beta \langle \beta | -\bar{R} \varepsilon_x |x >} \)

\( = -\varepsilon_x \varepsilon_\beta \langle \beta | \bar{R} |x > \)

\( \langle \beta | \bar{R} |x > = 0 \) unless \( \varepsilon_x = -\varepsilon_\beta \Rightarrow \)

\( \langle \beta | \bar{R} |x > \neq 0 \) only if \( 1x >, 1\beta > \) have opposite parity

\( \int \psi_\beta^* \bar{R} \psi_x \ d^2 \bar{r} = 0 \) if \( \psi_x, \psi_\beta \) are of the same parity

^ selection rule \( \Rightarrow \) used a lot in optics!